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Chaos and low-order corrections to classical mechanics or geometrical optics

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Based on simple first-order quantum corrections to classical equations of motion, which we show to be closely related to Gaussian wave-packet dynamics (GWD) and a time-dependent variational principle (TDVP), we deduce that quantum corrections to classical dynamics should typically become most pronounced when the classical system becomes chaotic. The time duration over which classical dynamics, GWD, or TDVP may provide good approximations is much shorter when the classical dynamics are chaotic. However, for certain situations involving very short laser pulses, these approximations can be very accurate. The same concepts are applicable to paraxial wave optics, which may offer simpler experimental studies of "quantum chaos": the distinction between classical and "quantum" chaos is in large part the distinction between ray versus wave behavior.

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I. INTRODUCTION

In this paper we employ an approximation to Heisenberg equations of motion to deduce conditions under which classical molecular dynamics can provide an accurate description of time-dependent quantum dynamics. Our approach involves a first-order cumulant approximation to the Heisenberg equations of motion, and is shown to give expectation values identical to those obtained by the method of Gaussian wave-packet dynamics (GWD) [1] for time-dependent problems. We deduce that all such methods equivalent to low-order cumulant expansions, including the simplest (zero-order) approximation of classical dynamics, are applicable over time scales that become shorter as the degree of sensitivity to initial conditions in the classical theory increases. Similar remarks apply to methods based on a time-dependent variational principle (TDVP) [2,3].

Cumulant expansions typically replace an infinite-dimensional system of equations by a finite number of equations, the zeroth-order approximation representing the classical dynamics and, as we shall see, the first-order approximation being closely related to the method of Gaussian wave-packet dynamics. Such expansions can also be employed in paraxial optics to obtain diffractive corrections to ray propagation, as we show in this paper. In fact, one purpose of this paper is to emphasize the close relation between classical versus quantum chaos and ray versus wave chaos. For instance, diffractive corrections to ray propagation can be expected to be most pronounced when the ray propagation is chaotic, just as quantum corrections to classical dynamics are typically most pronounced when the classical system is chaotic. Wave effects can be expected to suppress the chaos of ray propagation, just as quantum effects act to suppress classically chaotic time evolution.

In the following section our approach is described for the simplest class of system of interest to us that can exhibit chaos, namely, a one-dimensional nonlinear oscillator subject to a time-dependent force. We review a method for computing the maximal Lyapunov exponent for the classical system and compare the equations to be solved by this method to a first-order cumulant expansion of the Heisenberg equations of motion for the quantum system. We deduce in this way an important result obtained in a different way by Berman and Zaslavsky [4]: classical dynamics should typically provide an accurate approximation over shorter time scales when the corresponding classical system is chaotic than when it is regular, and in the classically chaotic regime the "crossover time" is on the order of the inverse of the maximal Lyapunov exponent. That is, the classical dynamics alone provide information as to the importance of quantum corrections. This is analogous to van Kampen's conclusion, based on a cumulant expansion of the master equation, that "the macroscopic stability ... determines whether or not the average of the [microscopic fluctuations] grows with time" [5].

In Secs. III and IV we show the connection of our approach to GWD and TDVP, respectively. The correlation between the transition to chaos in the classical dynamics and the breakdown of methods involving truncations in the cumulant equations or decorrelation is made explicit in Sec. V through a novel local stability analysis. Section VI considers three examples and contrasts the quantum and classical dynamics with the dynamics obtained when only the lowest-order quantum corrections are retained. Section VII describes the analogy between these considerations and paraxial optics, and our conclusions are summarized and discussed further in the final section.

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II. QUANTUM CORRECTIONS AND THE MAXIMAL LYAPUNOV EXPONENT

We begin with a classical system described by the Hamiltonian

$$H = \frac{p^2}{2m} + V(x) - xF(t) \,, \tag{1}$$

and review, based on this example, a method for computing the largest Lyapunov exponent of a system [6]. In the Hamilton equations $\dot{x} = p/m$ and $\dot{p} = -V'(x) + F(t)$ we replace $x(t)$ and $p(t)$ by $x(t) + \epsilon(t)$ and $p(t) + \eta(t)$ and retain terms only up to first order in the perturbations $\epsilon(t)$ and $\eta(t)$. That is, we consider the system of equations

$$\begin{aligned} \dot{x} &= p/m \,, \\ \dot{p} &= -V'(x) + F(t) \,, \\ \dot{\epsilon} &= \eta/m \,, \\ \dot{\eta} &= -V''(x)\epsilon \,. \end{aligned} \tag{2}$$

This system is integrated and along the way we compute

$$\chi(t) = \frac{1}{t} \ln \sqrt{\epsilon^2(t) + \eta^2(t)} \,, \tag{3}$$

where we choose the simplest measure of "distance" between trajectories, i.e., $\sqrt{\epsilon^2 + \eta^2}$. Then

$$\chi \equiv \lim_{t\to\infty} \chi(t) \,, \tag{4}$$

which turns out to be the largest Lyapunov exponent of the system, tells us whether the system is chaotic or regular. Specifically, the system is chaotic if $\chi > 0$ and regular otherwise. This is a standard definition of chaos for (deterministic) dynamical systems, and is the one assumed throughout this paper.

In general the value of χ, and therefore whether or not the system is chaotic, will depend on the initial point (x, p) of the phase space, whereas $\epsilon(0)$ and $\eta(0)$ can be given small but arbitrary values without generally affecting the computed value of χ [6]. As a practical matter the computation of χ will typically require large values of the integration time t before convergence is obtained. Note that $\epsilon(t)$ and $\eta(t)$ represent local perturbations to the trajectory $x(t), p(t)$; $\chi > 0$ implies an exponential separation, on average, of initially close trajectories.

Let us now turn to the quantum mechanics of the same system in the Heisenberg picture. It will be convenient to write the operators $X(t)$ and $P(t)$ as [7,8]

$$\begin{aligned} X(t) &= \langle X(t)\rangle + \delta X(t), \\ P(t) &= \langle P(t)\rangle + \delta P(t). \end{aligned} \tag{5}$$

We refer to δX and δP as "quantum corrections." Note that $\langle \delta X(t)\rangle$ and $\langle \delta P(t)\rangle$, by construction, are identically zero, and that

$$[\delta X(t), \delta P(t)] = i\hbar \tag{6}$$

in order that $[X(t), P(t)] = i\hbar$. The initial state vector $|\psi\rangle$ over which the expectation values $\langle X(t)\rangle$ and $\langle P(t)\rangle$ are taken is arbitrary, but the operators δX and δP are state dependent according to the definition (5). From the Heisenberg equations of motion $\dot{X} = P/m$ and $\dot{P} = -V'(X) + F(t)$ we have

$$\begin{aligned} \langle \dot{X}\rangle + \delta\dot{X} &= \frac{1}{m}\left(\langle P\rangle + \delta P\right), \\ \langle \dot{P}\rangle + \delta\dot{P} &= -V'(\langle X\rangle + \delta X) + F(t), \end{aligned} \tag{7}$$

or, using the fact that $\langle \delta X\rangle = \langle \delta P\rangle = 0$,

$$\begin{aligned} \langle \dot{X}\rangle &= \frac{1}{m}\langle P\rangle \,, \\ \langle \dot{P}\rangle &= -\langle V'(\langle X\rangle + \delta X)\rangle + F(t) \\ &= -V'(\langle X\rangle) + F(t) - \frac{1}{2}V'''(\langle X\rangle)\langle \delta X^2\rangle - \cdots, \\ \delta\dot{X} &= \frac{1}{m}\delta P, \\ \delta\dot{P} &= -V''(\langle X\rangle)\delta X - \frac{1}{2}V'''(\langle X\rangle)\left[\delta X^2 - \langle \delta X^2\rangle\right] - \cdots. \end{aligned} \tag{8}$$

Note that Eqs. (8) are identical to the first two of the classical equations (2), except for the quantum corrections involving $\langle \delta X^n\rangle$. If the quantum corrections are small in the sense that $|V'''(\langle X\rangle)|\langle \delta X^2\rangle$, etc. are small compared with $|-V'(\langle X\rangle) + F(t)|$, then Eqs. (8) reduce to the classical form

$$\begin{aligned} \langle \dot{X}\rangle &= \frac{1}{m}\langle P\rangle \,, \\ \langle \dot{P}\rangle &= -V'(\langle X\rangle) + F(t). \end{aligned} \tag{9}$$

If furthermore we ignore second- and higher-order quantum corrections in (8), then

$$\begin{aligned} \delta\dot{X} &= \frac{1}{m}\delta P \,, \\ \delta\dot{P} &= -V''(\langle X\rangle)\delta X. \end{aligned} \tag{10}$$

Now we note that Eqs. (9) and (10) have exactly the same form as Eqs. (2) determining the (classical) maximal Lyapunov exponent, although of course the equations (10) are operator equations. However, from (10) we obtain an infinity of c-number equations of which the first three are given by

$$\begin{aligned} \frac{d}{dt}\langle \delta X^2\rangle &= \frac{1}{m}\langle \delta X\delta P + \delta P\delta X\rangle \,, \\ \frac{d}{dt}\langle \delta X\delta P + \delta P\delta X\rangle &= \frac{2}{m}\langle \delta P^2\rangle - 2V''(\langle X\rangle)\langle \delta X^2\rangle \,, \\ \frac{d}{dt}\langle \delta P^2\rangle &= -V''(\langle X\rangle)\langle \delta X\delta P + \delta P\delta X\rangle, \end{aligned} \tag{11}$$

and these equations can be compared with the classical equations

$$\begin{aligned}\frac{d\epsilon^2}{dt} &= \frac{1}{m}(2\epsilon\eta),\\ \frac{d}{dt}(2\epsilon\eta) &= \frac{2}{m}\eta^2 - 2V''(x)\epsilon^2 ,\\ \frac{d\eta^2}{dt} &= -V''(x)(2\epsilon\eta),\end{aligned} \tag{12}$$

which follow from (2). The association

$$\begin{aligned}\epsilon^2 &\leftrightarrow \langle \delta X^2\rangle ,\\ 2\epsilon\eta &\leftrightarrow \langle \delta X\delta P + \delta P\delta X\rangle,\\ \eta^2 &\leftrightarrow \langle \delta P^2\rangle\end{aligned} \tag{13}$$

clearly puts (11) and (12) in the same form. Of course the two sets of equations are not really the same, because in (12) there are only two dependent variables whereas in (11) there are three. To restore consistency, one has to first remember that this apparent discrepancy is a consequence of the noncommutability of X and P. The property $[A,B] = iC$ implies

$$\langle A^2\rangle\langle B^2\rangle \geq \frac{1}{4}\left(\langle AB+BA\rangle^2 + \langle C\rangle^2\right), \tag{14}$$

which together with $[\delta X, \delta P] = i\hbar$ leads to $\langle \delta X^2\rangle\langle \delta P^2\rangle - (1/4)\langle \delta X\delta P + \delta P\delta X\rangle^2 = \text{const}$. In the classical limit, this reduces to $\langle \delta X^2\rangle\langle \delta P^2\rangle = (1/4)\langle \delta X\delta P + \delta P\delta X\rangle^2$ which makes the substitutions (13) consistent.

Suppose, then, that we describe a system classically and compute its maximal Lyapunov exponent using (2) or, equivalently, (12). If classical dynamics provide an accurate description of the system, we can anticipate that the quantum corrections satisfying (11) are small. When the classical dynamics become chaotic as some parameter is varied, however, the quantum corrections might be expected to grow, based on the similarity of (11) and (12). This conjecture will be explored in detail later in this paper.

It is worth noting that Eqs. (11) follow from the Heisenberg equations of motion with a Hamiltonian obtained by including quantum corrections up to second order:

$$\begin{aligned}H &= \frac{1}{2m}P^2 + V(X) - XF(t)\\ &\rightarrow \frac{1}{2m}\langle P\rangle^2 + V(\langle X\rangle) - \langle X\rangle F(t) + \frac{1}{2m}\delta P^2 - F(t)\delta X\\ &\quad + V'(\langle X\rangle)\delta X + \frac{1}{2}V''(\langle X\rangle)\delta X^2 - \cdots ,\end{aligned} \tag{15}$$

with $[\delta X, \delta P] = i\hbar$. The first three terms are c numbers and do not affect Heisenberg equations of motion, and so may be ignored for the purpose of obtaining the Heisenberg operator equations:

$$H \rightarrow \frac{1}{2m}\delta P^2 + V'(\langle X\rangle)\delta X - F(t)\delta X + \frac{1}{2}V''(\langle X\rangle)\delta X^2 . \tag{16}$$

Equations (11) for the lowest-order quantum corrections thus correspond to the approximation in which we follow the classical trajectories in phase space [Eqs. (9)] while assuming at every instant that the potential can be described *locally* by a simple quadratic form. The instantaneous quadratic potential determines our "quantum corrections" to lowest order.

III. QUANTUM CORRECTIONS AND GAUSSIAN WAVE-PACKET DYNAMICS

It is interesting to relate the "quantum corrections" construction to the method of GWD. Consider, following Heller [9], the example

$$H = \frac{P^2}{2m} + V(X) \tag{17}$$

and expand $V(X)$ about the classical trajectory x_t, p_t obtained from

$$\begin{aligned}\dot{x}_t &= p_t/m\\ \dot{p}_t &= -V'(x_t) ,\end{aligned} \tag{18}$$

leading to

$$V(X) = V(x_t) + V'(x_t)(X-x_t) + \frac{1}{2}V''(x_t)(X-x_t)^2 \tag{19}$$

when terms up to quadratic in $X - x_t$ are retained. Heller [9] assumes a Gaussian wave packet of the form

$$\psi(x,t) = e^{i[\alpha(x-x_t)^2 + p_t(x-x_t)+\gamma]} , \tag{20}$$

where $\alpha = \alpha_R + i\alpha_I$ and $\gamma = \gamma_R + i\gamma_I$ are complex and $\langle\psi|\psi\rangle = 1$. The time-dependent Schrödinger equation with the (time-dependent) potential (19) provides the differential equations satisfied by α, γ, x_t, and p_t:

$$\begin{aligned}\dot{x}_t &= \frac{p_t}{m} ,\\ \dot{p}_t &= -V'(x_t),\\ \dot{\alpha}_R &= -\frac{2}{m}(\alpha_R^2 - \alpha_I^2) - \frac{1}{2}V''(x_t),\\ \dot{\alpha}_I &= -\frac{4}{m}\alpha_R\alpha_I ,\\ \dot{\gamma} &= i\hbar\frac{\alpha}{m} + p_t\dot{x}_t - E,\end{aligned} \tag{21}$$

where $E = p_t^2/2m + V(x_t)$. It follows from (20) that

$$\begin{aligned}\langle X\rangle &= x_t ,\\ \langle P\rangle &= p_t ,\\ \langle X^2\rangle &= x_t^2 + \frac{1}{4\alpha_I} ,\\ \langle P^2\rangle &= p_t^2 + \frac{|\alpha|^2}{\alpha_I} ,\\ \langle \delta X\delta P + \delta P\delta X\rangle &= \frac{\alpha_R}{\alpha_I} ,\end{aligned} \tag{22}$$

so that $\langle \delta X^2\rangle = 1/4\alpha_I$ and $\langle \delta P^2\rangle = |\alpha|^2/\alpha_I$. These definitions together with (21) result in

$$\begin{aligned}\frac{d}{dt}\langle \delta X^2\rangle &= \frac{1}{m}\langle \delta X\delta P + \delta P\delta X\rangle ,\\ \frac{d}{dt}\langle \delta X\delta P + \delta P\delta X\rangle &= \frac{2}{m}\langle \delta P^2\rangle - 2\langle \delta X^2\rangle V''(x_t),\\ \frac{d}{dt}\langle \delta P^2\rangle &= -V''(x_t)\langle \delta X\delta P + \delta P\delta X\rangle .\end{aligned} \tag{23}$$

Thus the GWD method is analogous to including lowest-order quantum corrections to the classical evolution, except for the parameter γ. From (21) it is seen that the rate of change of γ_I is governed by the size of α_R which in turn reflects the importance of the quantum corrections. So with larger α_R, the imaginary part of γ grows (or decreases) faster and correspondingly adjusts the normalization of the wave packet, as seen from Eq. (20). This provides a mechanism for retaining the Gaussian form of the packet which in turn ensures the validity of the (time-dependent) quadratic form of the potential. In the extreme case where the quantum corrections grow rapidly, γ quickly damps away the maximum amplitude (at $x = x_t$) of the Gaussian, indicating the possible breakdown of the GWD approximation to the true dynamics. This is in contrast to the method of TDVP where the approximation defines a modified dynamics which may not bear any resemblance to the true dynamics [10].

IV. QUANTUM CORRECTIONS AND A TIME-DEPENDENT VARIATIONAL PRINCIPLE

When all the quantum-correction terms are included, Eqs. (9) become

$$\begin{aligned} \langle \dot{X} \rangle &= \frac{1}{m}\langle P \rangle \ , \\ \langle \dot{P} \rangle &= F(t) - \sum_{n=0}^{\infty} \frac{1}{n!} V^{(n+1)}(\langle X \rangle)\langle \delta X^n \rangle . \end{aligned} \tag{24}$$

In a time-dependent variational approximation the state of a system is assumed to stay in a general Gaussian form. In the Heisenberg picture this implies that n-point expectation values can be expressed in terms of one- and two-point expectation values. Following Pattanayak and Schieve [10], we employ the following relations under the *assumption* that the system at all times has the form of a "squeezed coherent state":

$$\begin{aligned} \langle \delta X^{2n} \rangle &= \frac{(2n)!}{n!2^n}\langle \delta X^2 \rangle^n \ , \\ \langle \delta X^{2n+1} \rangle &= 0, \\ \langle \delta X^2 \rangle \langle \delta P^2 \rangle &= \frac{1}{4}\hbar^2 + \frac{1}{4}\langle \delta X \delta P + \delta P \delta X \rangle^2 . \end{aligned} \tag{25}$$

Then (24) becomes

$$\begin{aligned} \langle \dot{X} \rangle &= \frac{1}{m}\langle P \rangle \ , \\ \langle \dot{P} \rangle &= F(t) - \sum_{n=0}^{\infty} \frac{1}{n!2^n} V^{(2n+1)}(\langle X \rangle)\langle \delta X^2 \rangle^n , \end{aligned} \tag{26}$$

and the evolution of $\langle \delta X^2 \rangle$ is fixed by the first of Eqs. (11):

$$\frac{d}{dt}\langle \delta X^2 \rangle = \frac{1}{m}\langle \delta X \delta P + \delta P \delta X \rangle \ . \tag{27}$$

For $\langle \delta X \delta P + \delta P \delta X \rangle$ we have

$$\begin{aligned} \frac{d}{dt}\langle \delta X \delta P + \delta P \delta X \rangle &= \frac{2}{m}\langle \delta P^2 \rangle - 2\sum_{n=1}^{\infty} \frac{1}{(n-1)!} V^{(2n)} \\ &\quad \times (\langle X \rangle)\langle \delta X^{2n} \rangle \\ &= \frac{\hbar^2 + \langle \delta X \delta P + \delta P \delta X \rangle^2}{2m\langle \delta X^2 \rangle} \\ &\quad - \sum_{n=1}^{\infty} \frac{V^{(2n)}(\langle X \rangle)}{(n-1)!2^{n-2}}\langle \delta X^2 \rangle^n \ , \end{aligned} \tag{28}$$

where we have used the ansatz (25).

The time-dependent variational equations for expectation values, Eqs. (26)–(28), have been obtained previously by Pattanayak and Schieve [10], who show that they reproduce the results based on the TDVP. Unlike the original quantum-correction hierarchy of equations, the TDVP equations form a closed set. For any potential $V(X)$, they form a *finite* (four) set of nonlinear equations and, as such, can exhibit chaos.

By defining a new pair of canonical variables $\rho^2 = \langle \delta X^2 \rangle$ and $\Pi = \langle \delta X \delta P + \delta P \delta X \rangle / 2\rho$, the four relations (26)–(28) can be recast as a two-dimensional Hamiltonian flow [10]. The corresponding effective Hamiltonian is

$$H_{eff} = \frac{p^2}{2m} + \frac{\Pi^2}{2m} + \frac{\hbar^2}{8m\rho^2} + \sum_{n=0}^{\infty} \frac{V^{2n}(x)}{n!2^n}\rho^{2n} - xF(t) \ , \tag{29}$$

where $p \equiv \langle P \rangle$ and $x \equiv \langle X \rangle$.

Pattanayak and Schieve [10] recently demonstrated that the "semiquantal" [2,3] dynamics described by this effective Hamiltonian for expectation values can be chaotic "even though the system has regular classical behavior and the quantum behavior had been assumed regular." This is counter to the usual expectation that quantum effects suppress classical chaos. However, their concluding remarks indicate caution in interpreting the semiquantal features as real. Our view of this situation, as discussed further in what follows, emphasizes the need for circumspection. We suggest that approximations such as GWD or TDVP are unreliable precisely when they or the completely classical equations exhibit features of chaos. The chaos should in our view be interpreted as symptomatic of the breakdown of the method (like numerical chaos) rather than as an independent phenomenon. However, as we shall also see, the generic form of the effective Hamiltonian (29) does provide some insight into the quantum suppression of classical hyperbolicity.

V. FAILURE OF LOW-ORDER QUANTUM CORRECTIONS AT THE TRANSITION TO CHAOS

Thus far our discussion has been restricted to either the lowest-order corrections to the classical evolution or decorrelating higher corrections as with the TDVP. We would now like to justify the statement that expansion schemes fail when the classical dynamics are chaotic. Working in the "extended" phase space of the modified

Heisenberg equations provides a compact way to see this effect.

Let us consider the dynamics in the vicinity of fixed points of the classical motion. As discussed in the Appendix, the extended phase space decouples into subspaces involving corrections of the same order. In the absence of quantum corrections, a local stability analysis would describe the local (classical) dynamics. The same prescription can be applied to the extended phase space where we first consider only the lowest-order corrections.

The fixed points are now given by

$$\begin{aligned} &\langle P\rangle = 0 \quad , \; V'(\langle X\rangle) = 0, \\ &\langle \delta X \delta P + \delta P \delta X\rangle = 0 \quad , \; \langle \delta P^2\rangle = V''(\langle X\rangle)\langle \delta X^2\rangle \; , \end{aligned} \tag{30}$$

where the first line is readily recognized as the defining relations for the classical fixed points. However, the solution for the quantum corrections depends on the curvature V'' of the potential, which also defines the character of the fixed point. For the stable or elliptic situation, $V'' > 0$, the coherent state or minimum uncertainty wave-packet condition for the widths,

$$\langle \delta X^2\rangle \sqrt{V''} = \frac{\langle \delta P^2\rangle}{\sqrt{V''}} \; , \tag{31}$$

is recovered. In the hyperbolic case where $V'' < 0$, the only consistent solution is $\langle \delta X^2\rangle = \langle \delta P^2\rangle = 0$. Similarly it can be shown that to the next order the second-order corrections are all zero at the fixed point.

The stability of the dynamics in the neighborhood of the fixed points is reflected in the eigenvalues of the local Jacobian or stability matrix. It is clear that within the quadratic approximation this matrix is block diagonal, which means the eigenvalues for each subspace of corrections can be obtained independently. Expressing the eigenvalues as exponents, in the $(\langle X\rangle, \langle P\rangle)$ subspace, these are

$$\lambda_0 = \pm\sqrt{-V''} \; , \tag{32}$$

while in the space of $(\langle \delta X^2\rangle, \langle \delta P^2\rangle, \langle \delta X \delta P + \delta P \delta X\rangle)$ one gets

$$\lambda_1 = 0, \; \pm 2\sqrt{-V''} \; , \tag{33}$$

where the derivative of the potential is to be evaluated at the fixed point. The zero exponent merely attests to the local Hamiltonian nature of the dynamics in the full five-dimensional space. Including the next higher-order corrections leads to a further four-dimensional subspace in which the exponents are now

$$\lambda_2 = \pm\sqrt{-V''} \; , \; \pm 3\sqrt{-V''} \; . \tag{34}$$

As seen from the Appendix, the third order brings in a five-dimensional subspace which requires, once again, that one of the exponents be zero in order to preserve a local Hamiltonian flow.

It is clear now that the stability in the extended phase space is governed entirely by the classical dynamics through the curvature of the potential V''. Near an elliptic fixed point, where the eigenvalues in the $(\langle X\rangle, \langle P\rangle)$ subspace are purely imaginary, harmonics of the classical circulation frequency appear in the space of quantum corrections. By contrast, near hyperbolic points, the subspace of quantum corrections for any order has a direction in which the corrections grow at a rate which is a multiple of the classical stretching rate [11]. Further, higher-order corrections grow at a faster rate than those of lower order.

Under the approximation of a quadratic potential, the decoupling of the extended phase space restricts the growth of any given order of corrections to its own subspace. Further, choosing a representation (like a coherent state) where the higher-order corrections are initially zero ensures that they remain zero for all times. However, this containment is lifted on including nonquadratic terms which mix the subspaces. The size of higher-order corrections is now governed by the lower-order ones as well which, as seen above, can then grow exponentially under certain conditions. Once the higher corrections are nonzero, they grow at a still faster rate. Together, these lead to the breakdown of methods involving cumulant expansions whenever the classical dynamics are unstable or chaotic. It is worth noting that in the elliptic case, inclusion of nonquadratic terms leads to harmonic generation in the extended space dynamics. This has long been a signature of anharmonic classical systems and has recently been the focus of both quantum-theoretic and experimental studies [12].

This demonstration provides the basis for the statement that quantum effects become more pronounced precisely when the classical dynamics are unstable or chaotic. The view then evolves that under these conditions, the infinite hierarchy of correlations must be dealt with. In lieu of confronting this infinite-dimensional system of first-order differential equations, it is more economical to resort to a partial differential equation, namely, the Schrödinger equation.

Knowing the fixed points of the dynamics in the "extended" phase space also leads to a novel inference, based simply on the form of the effective Hamiltonian (29) obtained within the TDVP [10]. This observation is particularly pertinent when the classical motion is unstable. First, we note that the contribution $\hbar^2/8\rho^2$ ($m = 1$ for simplicity) is common to all systems and results from the minimum uncertainty condition. Rewriting this term as $l_{min}^2/2\rho^2$, where $l_{min} = \hbar/2$ is the width of a minimum uncertainty packet, makes explicit the similarity with a centrifugal barrier where l_{min} is the effective "angular momentum." So, away from the classical limit, "s-wave" character is diminished with respect to the extended space variables.

As we saw earlier, a hyperbolic fixed point in the extended phase space requires $\langle X^2\rangle = \langle P^2\rangle = \langle \delta X \delta P + \delta P \delta X\rangle = 0$ which means $\rho = 0$. Thus the minimum uncertainty "centrifugal barrier" softens the hyperbolic character by screening the unstable fixed point in the extended phase space dynamics. In contrast, elliptic or stable fixed points (using minimum uncertainty conditions) require $\rho = \sqrt{\langle X^2\rangle} = \sqrt{\hbar/2} = \sqrt{l_{min}}$ which is

larger than l_{min} and thus is not affected by the presence of the barrier.

As the effective Hamiltonian is valid locally at least over some time, this behavior is generic to the neighborhood of all unstable and stable fixed points. Given that classical chaos is the byproduct of local instabilities associated with hyperbolic fixed points, the inference that quantum effects (finite $\hbar$) suppress chaos may be drawn. In terms of the extended phase space variables, two of which are classical and the other two quantum, this argument suggests a microscopic origin to the mechanism of quantum suppression.

VI. EXAMPLES

In order to briefly illustrate some of the points made in the foregoing discussion, we consider two nontrivial examples: a driven anharmonic oscillator model that does not exhibit chaos, and a driven Morse oscillator that does. We will contrast the exact quantum-mechanical results with both the purely classical dynamics and the dynamics including only the first-order quantum corrections (QC). First, however, we make a few remarks about the harmonic oscillator which, though trivial in the sense that the quantum corrections decouple from the evolution of the expectation values of X and P, nevertheless illustrates an important point.

For a harmonic oscillator of frequency ω_0 the solution to the time-dependent Schrödinger equation can be written in terms of energy (Fock) eigenstates $|n\rangle$ with expansion coefficients

$$C_n(t) = C_n(0)e^{-in\omega_0 t} , \tag{35}$$

from which the expectation value of any operator can be determined. For the initial state $|N\rangle$ with $C_n(0) = \delta_{n,N}$, for instance, the expectation values of the position operator

$$x = i\left(\frac{\hbar}{2m\omega_0}\right)^{1/2}(a - a^\dagger), \quad [a, a^\dagger] = 1 \tag{36}$$

and its square are given by

$$\begin{aligned}\langle x(t)\rangle &= i\left(\frac{\hbar}{2m\omega_0}\right)^{1/2}\langle N|(a - a^\dagger)|N\rangle = 0,\\ \langle x^2(t)\rangle &= \frac{\hbar}{m\omega_0}(N + 1/2) .\end{aligned} \tag{37}$$

For an initial coherent state $|\alpha\rangle$ with

$$C_n(0) = \frac{\alpha^n}{\sqrt{n!}}e^{-|\alpha|^2/2} \tag{38}$$

and $\alpha = r\exp(-i\theta)$, on the other hand,

$$\begin{aligned}\langle x(t)\rangle &= 2r\left(\frac{\hbar}{2m\omega_0}\right)^{1/2}\sin(\omega_0 t + \theta),\\ \langle x^2(t)\rangle &= \langle x(t)\rangle^2 + \frac{\hbar}{2m\omega_0} .\end{aligned} \tag{39}$$

The classical solution

$$x(t) = x_0\sin(\omega_0 t + \theta) , \quad x^2(t) = x_0^2\sin^2(\omega_0 t + \theta) , \tag{40}$$

which does not, of course, contain the zero-point energy, is in good agreement with the quantum coherent-state result for large $\langle n\rangle$, where the contribution from zero-point energy is negligible. However, to obtain good agreement with the quantum Fock state results, the classical solutions must be averaged over θ, in contrast to the deterministic classical analog for the coherent state. This exemplifies the usual microcanonical ensemble averaging employed in classical Monte Carlo methods when one attempts to mimic a quantum-mechanical energy eigenstate. The point here is that the Fock state and the coherent state have different classical statistical analogs, and each analog is equally "close" to its corresponding quantum state [13]. In fact, in the following examples we employ different classical statistical analogs, corresponding to a deterministic classical analog in the case of an initial coherent state and microcanonical ensemble averaging in the case of an energy eigenstate.

A. Driven anharmonic oscillator

Consider now the Hamiltonian

$$H = \omega_0 a^\dagger a - \chi(a^\dagger a)^2 + \Omega\left(ae^{i\omega t} + a^\dagger e^{-i\omega t}\right) , \tag{41}$$

where ω_0 is the natural frequency of the oscillator, χ controls the strength of the anharmonicity, Ω is the Rabi frequency which reflects the resonant coupling to the driving field, and ω is the frequency of the driving field. a and $a^\dagger$ are the usual annihilation and creation operators. The energy levels of the undriven system are simply

$$E_n = n\omega_0 - n^2\chi , \quad n = 0, 1, 2, \ldots . \tag{42}$$

The fact that the unperturbed Hamiltonian is not bounded from below does not pose any practical difficulty provided the excitation probability of states with $E_n < 0$ is negligible.

Once again we write the full quantum solution $\Psi(t)$ within the oscillator basis, that is,

$$\Psi(t) = \sum_n C_n(t)e^{-in\omega t}|n\rangle . \tag{43}$$

From the time-dependent Schrödinger equation, the amplitudes $C_n(t)$ evolve according to

$$\begin{aligned}\dot{C}_n(t) = &-i(n\Delta - n^2\chi)C_n(t)\\ &-i\Omega\sqrt{n+1}C_{n+1}(t) - i\Omega\sqrt{n}C_{n-1}(t) ,\end{aligned} \tag{44}$$

where the detuning $\Delta = \omega_0 - \omega$. The expectation value of the number operator is simply

$$\langle n(t)\rangle = \sum_{n=0}^{\infty} n|C_n(t)|^2 . \tag{45}$$

Classically, the evolution of the complex amplitude is given by

$$\dot{a}(t) = -i(\omega_0 - \chi)a(t) + i2\chi|a(t)|^2 a(t) - i\Omega e^{-i\omega t} , \quad (46)$$

which, writing $a(t) = \alpha(t)e^{-i\omega t}$, becomes

$$\dot{\alpha}(t) = -i(\Delta - \chi)\alpha(t) + i2\chi|\alpha(t)|^2\alpha(t) - i\Omega , \quad (47)$$

from which

$$n_{cl}(t) = |\alpha(t)|^2 . \quad (48)$$

To add quantum corrections to the classical dynamics, we begin with the Heisenberg equation of motion for a:

$$\dot{a} = -i[a, H] = -i(\Delta - \chi)a + i2\chi a^\dagger aa - i\Omega . \quad (49)$$

We now let $a = \langle a\rangle + \delta a \equiv \alpha + \delta a$. It is clear from the definition that $\langle \delta a\rangle = 0$. Denoting the lowest-order quantum corrections by $x_1 = \langle \delta a \delta a\rangle$ and $x_2 = \langle \delta a^\dagger \delta a\rangle$, we have, in the extended space (α, x_1, x_2), the three evolution equations

$$\begin{aligned}
\dot{\alpha} &= -i(\Delta - \chi)\alpha + i2\chi|\alpha|^2\alpha - i\Omega + i2\chi[\alpha^* x_1 + 2\alpha x_2] , \\
\dot{x_1} &= -i2(\Delta - \chi)x_1 + i8\chi|\alpha|^2 x_1 + i4\chi\alpha^2 x_2 + i2\chi\alpha^2 , \\
\dot{x_2} &= i2\chi(\alpha^2 x_1^* - \alpha^{*2} x_1) .
\end{aligned} \quad (50)$$

The expectation value of the number operator is now given by

$$n_{cl+qc}(t) = |\alpha|^2 + x_2 . \quad (51)$$

These relations explicitly display the coupling of higher- and lower-order corrections via the anharmonicity, which also governs the importance of the corrections.

The evolution of the amplitudes can be numerically solved for each case and the total energy, which is the expectation value of the number operator, can be computed as a function of time. This is shown in Fig. 1 for three cases exploring different aspects of the dynamics. Figure 1(a) corresponds to weak anharmonicity, small detuning, and modest Rabi frequency. It is seen that for times on the order of a few cycles, the agreement between classical, quantum-mechanical, and QC dynamics is very good. It can also be seen that the QC dynamics agree with the full quantum dynamics for a longer duration than the classical dynamics. The same is true in Fig. 1(b), which shows a resonant case ($\Delta = 0$) with large anharmonicity and large Rabi frequency. This is, of course, a case where the anharmonicity makes it essentially a strongly driven two-level dynamics. Both classical and QC dynamics deviate from the full quantum evolution at approximately the same point for the last case [Fig. 1(c)], which has a very weak anharmonic component, large detuning, and a substantial Rabi coupling.

These results are not unexpected: quantum corrections allow us to extend the range of time over which reasonably good agreement with the full quantum dynamics can be obtained. However, the classical system does not admit the possibility of chaos. We now consider an example where chaos can occur in the classical dynamics.

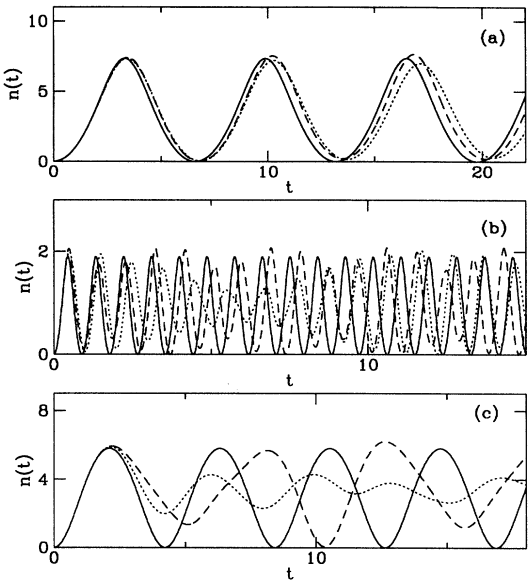

FIG. 1. Comparison of the quantum expectation value of the number operator $\langle n(t)\rangle$ (dotted line) with both the classical energy $n_{cl}(t)$ (solid line) and $n_{cl+qc}(t)$ (dashed line) calculated by including lowest-order quantum corrections. Parameter values considered were (a) $\Omega = 1.0$, $\chi = 0.1$, and $\Delta = 0.1$; (b) $\Omega = 4.0$, $\chi = 2.0$, and $\Delta = 0.0$; (c) $\Omega = 2.0$, $\chi = 0.05$, and $\Delta = 2.0$.

B. Driven Morse oscillator

The Morse potential has traditionally been useful in the analysis of vibrational spectra of diatomic molecules. In recent years both classical and quantum versions of the driven Morse oscillator have been featured in a wide range of studies [14,15]. For our purposes, it is enough to note that issues of chaos and quantum-classical correspondence have been addressed by studies of photodissociation within the Morse system [15].

The Hamiltonian for the driven Morse potential is

$$H = \frac{p^2}{2m} + D(1 - e^{-ax})^2 - d_1 E_0 x \cos\omega t , \quad (52)$$

where D and a provide the energy and length scales, respectively, for the Morse potential. These also determine the frequency $\omega_0 = (2Da^2/m)^{1/2}$ of the approximately harmonic motion near the bottom of the well. d_1 is the dipole gradient. We introduce the variables

$$\begin{aligned}
B &= \left(\hbar^2 a^2/2mD\right)^{1/2} , \\
\tau &= \left(DB^2/\hbar\right) t , \\
X_{sc} &= ax , \\
P_{sc} &= p/\hbar a , \\
\mu &= \hbar\omega/DB^2 , \\
K &= d_1 E_0/aDB^2 ,
\end{aligned} \quad (53)$$

in terms of which the classical equations of motion are

$$\dot{X}_{sc} = 2P_{sc},$$
$$\dot{P}_{sc} = -(2/B^2)(e^{-X_{sc}} - e^{-2X_{sc}}) + K\cos\mu\tau\ , \tag{54}$$

where the derivative is now with respect to τ. The energy is now expressed in units of the dissociation energy D. As the initial state for the quantum theory is an energy eigenstate, we follow the usual procedure of considering a microcanonical ensemble of initial conditions, solving the equations of motion and then computing the ensemble averaged energy E.

For the full quantum dynamics, we numerically solve the Schrödinger equation

$$i\frac{\partial\psi}{\partial\tau} = -\frac{\partial^2\psi}{\partial X_{sc}^2} + B^{-2}(1-e^{-X_{sc}})^2\psi - KX_{sc}\cos\mu\tau\psi \tag{55}$$

on a space-time grid using a standard method [16]. From the wave function, the time-dependent expectation value of E is constructed and compared with its classical counterpart.

On adding the first-order quantum corrections, which we denote by $u = \langle\delta X^2\rangle$, $v = \langle\delta P^2\rangle$, and $w = \langle\delta X\delta P + \delta P\delta X\rangle$, we get the coupled equations

$$\begin{aligned}
\frac{d}{d\tau}\langle X\rangle &= 2\langle P\rangle\ ,\\
\frac{d}{d\tau}\langle P\rangle &= -\frac{2}{B^2}(e^{-\langle X\rangle} - e^{-2\langle X\rangle}) + K\cos\mu\tau\\
&\quad -\frac{1}{B^2}(e^{-\langle X\rangle} - 4e^{-2\langle X\rangle})u\ ,
\end{aligned} \tag{56}$$

$$\begin{aligned}
\frac{d}{d\tau}u &= 2w\ ,\\
\frac{d}{d\tau}v &= -\frac{2}{B^2}(2e^{-2\langle X\rangle} - e^{-\langle X\rangle})w\ ,\\
\frac{d}{d\tau}w &= 4\left[v - \frac{u}{B^2}(2e^{-2\langle X\rangle} - e^{-\langle X\rangle})\right]\ ,
\end{aligned}$$

which are solved numerically. The initial conditions are those obtained from the wave functions for the undriven Morse potential (see [15] for details). To this order the energy is given by

$$\frac{E_{cl+qc}}{D} = B^2[\langle P\rangle^2 + v] + (1-e^{-\langle X\rangle})^2 + (2e^{-2\langle X\rangle} - e^{-\langle X\rangle})u\ . \tag{57}$$

The effective Hamiltonian (semiquantal) resulting from the TDVP also has a nicely closed form for the Morse potential. Summing over the derivatives of the potential in (29) and changing to the scaled variables we have

$$H_{eff} = P^2 + \Pi^2 - K\cos\mu\tau X + \frac{1}{\rho^2} + \frac{1}{B^2}\left[1 - 2e^{-X}e^{\rho^2/2} + e^{-2X}e^{2\rho^2}\right]\ , \tag{58}$$

from which follow the coupled differential equations

$$\begin{aligned}
\frac{d}{d\tau}X &= 2P\ ,\\
\frac{d}{d\tau}P &= -\frac{2}{B^2}(e^{-X+\rho^2/2} - e^{-2X+2\rho^2}) + K\cos\mu\tau\ ,\\
\frac{d}{d\tau}\rho &= 2\Pi\ ,\\
\frac{d}{d\tau}\Pi &= \frac{1}{2\rho^3} + \frac{2\rho}{B^2}(e^{-X+\rho^2/2} - 2e^{-2X+2\rho^2})\ .
\end{aligned} \tag{59}$$

These four equations can be integrated starting with the same initial conditions as for Eqs. (56). Now we are ready to make a comparison of these four distinct dynamics.

In the choice of parameters, we are assisted by the knowledge that classical chaos becomes more relevant as the probability for dissociation increases [15]. Thus we should contrast the dynamics described by Eqs. (54)–(56) for cases of large and small dissociation probabilities.

In Fig. 2 we display two cases discussed by Goggin and Milonni [15]. The first involves strong driving and the scaled frequency μ is tuned away from the $n = 0 \to 1$ quantum resonance. The classically computed energy deviates after a few cycles from the quantum mechanically computed energy, while the QC dynamics remain accurate for ≈ 10 optical cycles. The TDVP tracks the true quantum dynamics for a shorter time than the truncated QC dynamics though it does provide an improvement over the classical dynamics. This comparison between the TDVP and QC dynamics holds for the case shown in Fig. 2(b) with weaker driving field but with the frequency tuned to the $n = 0 \to 1$ resonance. The classical dynamics are more regular in this case and the QC dynamics once again agree with the quantum dynamics for almost twice as long as in the case of Fig. 2(a). The implications of these results are discussed further in Sec. VIII.

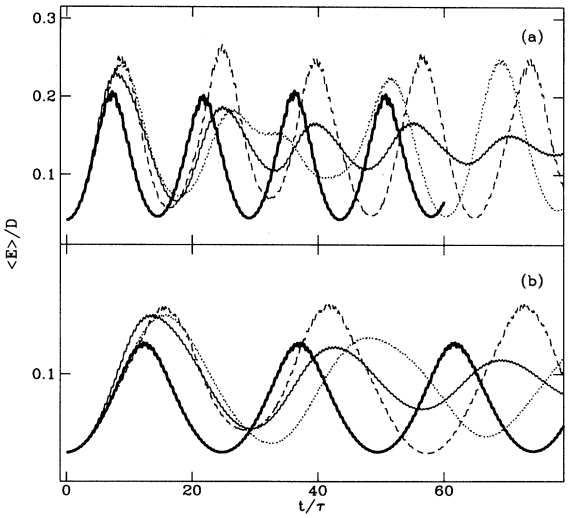

FIG. 2. Comparison of the dimensionless energy (scaled to the dissociation energy) computed from the quantum (dotted), classical (thin solid), lowest-order QC (dashed), and TDVP or semiquantal (thick solid) dynamics. Parameter values are (a) $K = 23.7$ and $\mu = 45.11$; (b) $K = 10.0$ and $\mu = 45.73$. Time is measured in units of optical cycles τ.

VII. PARAXIAL OPTICS IN "QUANTUM-MECHANICAL" FORM

Questions of "quantum chaos" can be posed within the framework of purely classical theory, whenever there is a ray (trajectory) approximation to fundamentally wavelike behavior. In this sense the distinction between classically chaotic behavior and quantum mechanically regular behavior is more aptly characterized as a distinction between ray and wave propagation. Quantum corrections to classical dynamics are then analogous to diffractive corrections to ray propagation. This section illustrates this point in the context of purely classical paraxial wave optics.

Maxwell's equations for media with no net charge or current imply the equation

$$\nabla^2\mathbf{E}+\epsilon\frac{\omega^2}{c^2}\mathbf{E}+\nabla\left(\frac{1}{\epsilon}\nabla\epsilon\cdot\mathbf{E}\right)=0 \tag{60}$$

for the electric field $\mathbf{E}(\mathbf{r})e^{-i\omega t}$. If $\epsilon\cong 1$ and if variations in $\epsilon(\mathbf{r})$ are sufficiently small, the third term on the left side of Eq. (60) can be ignored and we can work with the Helmholtz equation

$$\nabla^2E+k^2n^2(\mathbf{r})E=0, \tag{61}$$

where $k=\omega/c$ and $n^2=\epsilon$, for each scalar component of the field. In the paraxial approximation we write

$$E(\mathbf{r})=E_0(\mathbf{r})e^{ikz} \tag{62}$$

and assume that variations of E_0 with respect to z are small on a scale of a wavelength $(2\pi/k)$. This leads to the well known paraxial wave equation [17]

$$2ik\frac{\partial E_0}{\partial z}=-\nabla_T^2E_0-(n^2-1)E_0\ , \tag{63}$$

or

$$i\frac{\partial E_0}{\partial z}=-\frac{1}{2k}\nabla_T^2E_0-kn_1E_0 \tag{64}$$

for $n^2\cong 1$, i.e., $n^2-1\cong 2(n-1)\equiv 2n_1$.

Equation (64) has exactly the same form as the time-dependent Schrödinger equation when the substitutions $t\to z$, $\hbar\to 1$, $m\to k$, and $V\to -kn_1$ are made in the latter. Of course we can cast the paraxial wave equation (64) in the language of bras, kets, and a linear vector space of square-integrable functions [18]:

$$i\frac{\partial}{\partial z}|E_0\rangle=\left[\frac{\mathbf{p}^2}{2k}+kn_1(\mathbf{r})\right]|E_0\rangle, \tag{65}$$

with $[r_i,p_j]=i\delta_{ij}$. We can also define a Hamiltonian

$$H=\frac{\mathbf{p}^2}{2k}+kn_1(\mathbf{r})\ , \tag{66}$$

in terms of which (65) represents the "time-dependent" Schrödinger equation. With this Hamiltonian we can also work in the Heisenberg representation where

$$\frac{d\mathbf{r}}{dz}=\frac{1}{i}[\mathbf{r},H]=\frac{\mathbf{p}}{k}\ , \tag{67}$$

$$\frac{d\mathbf{p}}{dz}=\frac{1}{i}[\mathbf{p},H]=-k\nabla n_1\ . \tag{68}$$

It follows from these "Heisenberg equations of motion" that

$$\frac{d^2\mathbf{r}}{dz^2}=\nabla n_1\ , \tag{69}$$

which is the paraxial approximation to the ray equation $(d/ds)(nd\mathbf{r}/ds)=\nabla n_1$, $n\cong 1$, for a position vector $\mathbf{r}$ of a point on a ray, with s a distance measured along the ray [19]. In our formulation Eqs. (65)–(67) are equations of motion for operators in a Hilbert space, and "quantum" corrections are actually diffractive corrections to ray propagation. The initial state over which the rays and the diffractive corrections are calculated is $|E_0(0)\rangle$, i.e., $E_0(x,y,z=0)$.

The effective "quantum dynamics" associated with the paraxial wave equation has been exploited by various authors [20], and optical analogs of harmonic oscillators, two-level atoms, stabilization, and other "quantum" systems have been discussed previously [21]. The point of interest here is that, if the refractive index $n_1(\mathbf{r})$ is such as to give nonlinear equations and chaos in the ray approximation, then the effect of diffraction (wave optics) will be to suppress this chaotic behavior, in complete analogy to the suppression of classical chaos in quantum mechanics. We can introduce "diffractive corrections" to ray optics in exact correspondence to the quantum corrections to classical dynamics; the ray approximation, or the ray approximation with low-order diffractive corrections, will typically be accurate for short propagation distances, just as classical dynamics will typically be adequate on short time scales. When the rays propagate chaotically, however, diffractive effects can be expected to become important for shorter distances of propagation than in the case of regular ray propagation, just as quantum corrections in the case of classical chaos become important, typically, for shorter times than in the case of regular classical dynamics.

It is perhaps worth noting that the analogy between the paraxial wave equation and the time-dependent Schrödinger equation carries through especially clearly in the special case of quantum systems in which only a few energy levels are relevant (e.g., two-level atoms). In particular, consider

$$n_1(\mathbf{r})=n_1^{(0)}(x,y)+A(x,y)\cos\Omega z \tag{70}$$

and the expansion

$$E_0(x,y,z)=\sum_n a_n(z)G_n(x,y)e^{-iK_nz}, \tag{71}$$

where the $G_n(x,y)$ are the eigenfunctions for the unperturbed optical system defined by

$$-\frac{1}{2k}\nabla_T^2G_n(x,y)-kn_1^{(0)}(x,y)G_n(x,y)=K_nG_n(x,y), \tag{72}$$

and the K_n are the corresponding eigenvalues. Then Eqs. (70)–(72) imply

$$i\frac{da_n}{dz} = -k\cos\Omega z \sum_m X_{nm} a_m(z) e^{-i(K_m - K_n)z} , \quad (73)$$

where we have invoked the orthogonality of the eigenfunctions $G_n(x,y)$ and have defined

$$X_{nm} = \int\int dxdy G_n^*(x,y) A(x,y) G_m(x,y). \quad (74)$$

We are assuming that the unperturbed optical system is lossless, and so defines a Hermitian eigenvalue problem with a complete orthogonal set of eigenfunctions.

Suppose, for instance, that the mode $G_1(x,y)$ is injected at $z = 0$ into the system described by Eq. (72). Then, if $\Omega \cong K_2 - K_1$ is significantly different from all the other $K_m - K_1$, we are led to the approximation that only the modes $G_1(x,y)$ and $G_2(x,y)$ are coupled by the perturbation represented by the second term in Eq. (70). This "two-level" approximation reduces (73) to the system

$$\frac{da_1}{dz} = i\Omega_R a_2 , \quad \frac{da_2}{dz} = i\Omega_R a_1 , \quad (75)$$

where we assume that the "Rabi frequency" $\Omega_R \equiv \frac{1}{2}kX_{12}$ is real. Then

$$|a_1(z)|^2 = \cos^2\Omega_R z , \quad |a_2(z)|^2 = \sin^2\Omega_R z , \quad (76)$$

i.e., the two modes exhibit "Rabi oscillations" as they propagate through the system.

One can envision a large number of other "quantum-mechanical" effects in the paraxial propagation of light [22,23]. Such optical analogies include effects associated with different "quantum" states of, say, the simple harmonic oscillator. The Hermite-Gaussian modes of a stable laser resonator, for instance, correspond to eigenstates of a two-dimensional harmonic oscillator, and if a linear combination of these modes with expansion coefficients of the type (38) could be realized we would have a coherent state in which the centroid $\langle \mathbf{r}(z) \rangle$ of the transverse field pattern oscillates harmonically, corresponding to a scanning beam. In fact, a sufficiently large number of modes ($\cong 7$) were coupled in phase, resulting in a scanning beam, in experiments conducted many years ago by Auston [24].

VIII. DISCUSSION

Using a cumulant expansion of the Heisenberg equations of motion for quantum-mechanical operators, we have shown how to obtain "quantum corrections" to purely classical equations of motion. These quantum corrections follow equations of motion that couple them not only to the classically determined variables, but also to higher-order quantum corrections, so that the expectation value of any quantum-mechanical operator can be obtained at any time t by solving a sufficiently large number of coupled first-order ordinary differential equations. The initial conditions for these differential equations are determined by expectation values over the initial state of the system.

By noting the similarity between the coupled equations for the classical canonical variables, and the quantum corrections up to first order, to the equations determining the maximal Lyapunov exponent of the classical system, we have deduced an important conclusion concerning the relative importance of quantum corrections in classically regular and classically chaotic systems: The quantum corrections should typically grow much faster in time when the classical system is chaotic than when it is regular. In addition, higher-order quantum corrections should grow more rapidly compared with lower-order ones when the classical system is chaotic than when it is regular. Since Gaussian wave-packet dynamics have been shown to be closely related to equations of motion including quantum corrections through only first order (Sec. III), one anticipates that this approximation will not in general be reliable for strongly chaotic systems. Similarly, results based on a time-dependent variational principle (Sec. IV) cannot be expected to be reliable in general when the corresponding classical system exhibits chaos.

It has been shown that starting from a more general form for the wave packet, which requires information beyond the first two moments, leads to a generalization of GWD [25]. It would appear reasonable to expect that this construction is equivalent to including higher-order quantum corrections in our method.

Purely classical dynamics provide a measure of when quantum effects are most likely to be important, just as macroscopic stability properties can determine the growth of microscopic fluctuations in purely classical systems [5].

While it is difficult in general to deduce a precise "break time" at which classical dynamics are a poor approximation for chaotic systems, our simple analysis suggests that this time is roughly on the order of the inverse of the largest Lyapunov exponent, in agreement with Berman and Zaslavsky [4].

Our conclusions bode ill for the general reliability of classical molecular dynamics or simple GWD or TDVP approximations in classically chaotic systems. However, it should be borne in mind that there is generally *some* time over which these approximations *are* accurate, if the classical statistical analog is chosen properly (Sec. VI), i.e., in such a way that the classical and quantum-mechanical averages are in close correspondence at $t = 0$. The results for the Morse oscillator, for instance, suggest that, except for extremely intense fields, classical molecular dynamics should make reliable predictions at least over several cycles of an applied laser field. We therefore expect that classical approximations, GWD, or TDVP methods will be very useful in the study of molecular systems irradiated by femtosecond probe pulses. In fact, the predictions of classical molecular dynamics have been found to be a very useful guide in the short-pulse photodissociation dynamics of alkali halides [26].

It should be noted that the simple method of quantum corrections can be useful even in certain situations

where the system, or part of the system, has no obvious classical analog. In such situations the "quantum corrections" provide a measure of the accuracy of decorrelation approximations. Shirley [8], for instance, has employed essentially just this method in a study of the validity of the semiclassical approximation in laser theory. In this case the system consists of a collection of two-level atoms coupled to the electromagnetic field, and what we have termed "quantum corrections" account for corrections to the approximation of decorrelating atomic and field variables. In other words, the calculation of quantum corrections can provide a straightforward and very useful quantitative estimate of "mean field" and other decorrelation procedures.

In this paper we have also emphasized the analogy between paraxial wave optics and time-dependent quantum-mechanical phenomena, and in particular that questions of quantum chaos can be studied within the context of purely classical paraxial optics. The short-time validity of classical dynamics or classical dynamics with low-order quantum corrections is analogous to the fact that ray-optical propagation—or ray-optical propagation with low-order diffractive corrections—can provide a good approximation for short propagation distances. Thus, in the context of chaos as well as other phenomena, Gabor's remark that "quantum mechanics is not a bad preparation for optics" [27] is worth remembering.

Note added in proof. Gaussian wave-packet techniques have recently been extended to obtain agreement with quantum-mechanical results over time intervals greater than the "log time." See, for instance, M. A. Sepulveda, S. Tomsovic, and E. J. Heller, Phys. Rev. Lett. **69**, 402 (1992).

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APPENDIX: EVOLUTION EQUATIONS FOR HIGHER-ORDER QUANTUM CORRECTIONS

For the sake of completeness we list the evolution equations satisfied by quantum corrections up to fourth order. Note that we use these only for the stability analysis, in extended phase space, in the neighborhood of the classical fixed points. As a consequence, we *display here only terms up to the first nonquadratic contribution from the potential* (i.e., the triple derivative).

To fourth order in quantum corrections, there are 14 coupled equations:

$$\begin{aligned}
\frac{d\langle X\rangle}{dt} &= \langle P\rangle \,, \\
\frac{d\langle P\rangle}{dt} &= -V' - \frac{V'''}{2}\langle \delta X^2\rangle + F(t),
\end{aligned} \tag{A1}$$

$$\begin{aligned}
\frac{d}{dt}\langle \delta X^2\rangle &= \langle \delta X \delta P + \delta P \delta X\rangle \,, \\
\frac{d}{dt}\langle \delta P^2\rangle &= -V''\langle \delta X \delta P + \delta P \delta X\rangle - V'''\langle \delta X \delta P \delta X\rangle \,, \\
\frac{d}{dt}\langle \delta X \delta P + \delta P \delta X\rangle &= 2\langle \delta P^2\rangle - 2V''\langle \delta X^2\rangle - V'''\langle \delta X^3\rangle,
\end{aligned} \tag{A2}$$

$$\begin{aligned}
\frac{d}{dt}\langle \delta X^3\rangle &= 3\langle \delta X \delta P \delta X\rangle \,, \\
\frac{d}{dt}\langle \delta P^3\rangle &= -3V''\langle \delta P \delta X \delta P\rangle + V'''\left(\frac{3}{2}\langle \delta X^2\rangle\langle \delta P^2\rangle - \frac{3}{2}\langle \delta P \delta X^2 \delta P\rangle + \hbar^2\right) \,, \\
\frac{d}{dt}\langle \delta X \delta P \delta X\rangle &= 2\langle \delta P \delta X \delta P\rangle - V''\langle \delta X^3\rangle - \frac{V'''}{2}\left(\langle \delta X^4\rangle - \langle \delta X^2\rangle^2\right) \,, \\
\frac{d}{dt}\langle \delta P \delta X \delta P\rangle &= \langle \delta P^3\rangle - 2V''\langle \delta X \delta P \delta X\rangle + \frac{V'''}{2}\left(\langle \delta X^2\rangle\langle \delta X \delta P + \delta P \delta X\rangle - \langle \delta X^3 \delta P + \delta P \delta X^3\rangle\right) \,,
\end{aligned} \tag{A3}$$

$$\begin{aligned}
\frac{d}{dt}\langle \delta X^4\rangle &= 2\langle \delta X^3 \delta P + \delta P \delta X^3\rangle \,, \\
\frac{d}{dt}\langle \delta P^4\rangle &= -2V''\langle \delta X \delta P^3 + \delta P^3 \delta X\rangle + 2V'''\langle \delta X^2\rangle\langle \delta P^3\rangle \,, \\
\frac{d}{dt}\langle \delta X^3 \delta P + \delta P \delta X^3\rangle &= -2V''\langle \delta X^4\rangle - 3\hbar^2 + 6\langle \delta P \delta X^2 \delta P\rangle + V'''\langle \delta X^2\rangle\langle \delta X^3\rangle \,, \\
\frac{d}{dt}\langle \delta X \delta P^3 + \delta P^3 \delta X\rangle &= 2\langle \delta P^4\rangle + 3V''\left(\hbar^2 - 2\langle \delta P \delta X^2 \delta P\rangle\right) + 3V'''\langle \delta X^2\rangle\langle \delta P \delta X \delta P\rangle \,, \\
\frac{d}{dt}\langle \delta P \delta X^2 \delta P\rangle &= -V''\langle \delta X^3 \delta P + \delta P \delta X^3\rangle + \langle \delta P^3 \delta X + \delta X \delta P^3\rangle + V'''\langle \delta X^2\rangle\langle \delta X \delta P \delta X\rangle \,.
\end{aligned} \tag{A4}$$

Note that all derivatives of the potential are evaluated at $\langle X \rangle$. It is clear that under the quadratic approximation, the evolution decouples into closed subspaces involving variables of the same order. Thus the first three orders of quantum corrections involve three, four, and five variables, respectively. This decoupling is especially effective in the neighborhood of fixed points of the classical dynamics where the quadratic approximation is particularly good. This motivates the local stability analysis used earlier to correlate classical instability with the growth of quantum corrections. It should be noted that equations for higher-order corrections were included in Ref. [28] but truncating those to V''' does not yield (A4). This is because the relations in Ref. [28] are not entirely self-consistent.

It might appear that the truncation of the equations for higher-order moments is somewhat arbitrary, given the infinity of correlation functions generated. However, for time-dependent systems, the requirement that $dH/dt = 0$ in the absence of the driving term provides a systematic procedure [29] for deciding which terms need be retained to preserve energy conservation to a certain order of corrections (or alternately, derivative of the potential).

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